## TURBULENT MASS TRANSFER WITH FIRST ORDER CHEMICAL REACTION

## Bojan M. Mitrovic<sup>a</sup> and Dimitrios V. Papavassiliou<sup>b</sup>

<sup>a</sup>Department of Chemical Engineering & Materials Science The University of Oklahoma Norman, Oklahoma 73019 boxyusa@yahoo.com

bDepartment of Chemical Engineering & Materials Science Sarkeys Energy Center The University of Oklahoma Norman, Oklahoma 73019 dvpapava@ou.edu

This work examines the mass transfer properties for the case of turbulent transport with 1st order chemical reaction. Numerical experiments using a direct numerical simulation (DNS) of turbulent flow in a channel, combined with Lagrangian scalar tracking (LST) of trajectories of mass markers in the flow field [1,2,3] are conducted. The probability density function that describes the behavior of an instantaneous heat or mass source at the wall of the channel is used to synthesize the mean concentration profile of a reactant that is dissolved in the flow field from one wall of the channel. A second probability function, one that depends on the rate of a first order chemical reaction, is used to determine which markers react as time advances.

It is found that the mass transfer coefficient for the reactant increases, especially for fast reactions. The range of Schmidt numbers examined is between  $1 \times 10^{-1}$  and  $5 \times 10^{4}$ , and the range of Damköhler numbers is between  $1.4 \times 10^{-2}$  and  $1.4 \times 10^{-4}$ . Quantitative relations are developed to predict the dependence of the mass transfer coefficient on the Damköhler number and on the Schmidt number. Results from the DNS/LST method are compared to existing data and to results from the modeling of mass transfer based on the analogy between mass and momentum transfer in turbulent flow. It is argued that differences from what the analogy predicts are due to (a) the presence of the wall, which results to an effective filtering of the size of the eddies that contribute to turbulent transport depending on the molecular Schmidt number of the fluid, and (b) the amount of time that is necessary for a mass marker to be transferred out of the viscous wall layer relative to the reaction half-life time.

## References

- [1] Papavassiliou, D.V., and T.J. Hanratty, "Transport of a passive scalar in a turbulent channel flow", *Int. J. Heat Mass Transfer*, **40**(6), p. 1303-1311, 1997.
- [2] Papavassiliou, D.V, "Turbulent transport from continuous sources at the wall of a channel," *Int. J. Heat Mass Transfer*, **45**(17), p. 3571-3583, 2002.
- [3] Mitrovic B.M., and D.V. Papavassiliou, "Transport properties for turbulent dispersion from wall sources," in press, *AIChE Journal*, 2003.